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("Time-Advance Algorithms Based on Hamilton's
Principle")

Covering the Period 1 August 1992 to 30 September 1995

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Summary

Hamilton's principle was applied to derive a class of numerical algorithms for systems of ordinary differential equations when the equations are derivable from a Lagrangian. This is an important extension into the time domain of an earlier use of Hamilton's principle to derive algorithms for the spatial operators in Maxwell's equations. In that work, given a set of expansion functions for spatial dependences, the Vlasov-Maxwell equations were replaced by a system of ordinary differential equations in time; but the question of solving the ordinary differential equations was not addressed. Advantageous properties of the new time-advance algorithms were identified analytically and by numerical comparison with other methods, such as Runge-Kutta and symplectic algorithms. This approach to time advance can be extended to include partial differential equations and the Vlasov-Maxwell equations. Application has been made to derive a second-order accurate algorithm for the linear wave equation; the dispersive properties of the algorithm are superior to those of the usual second-order accurate explicit or implicit algorithms.

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Introduction

In the description of plasmas and other systems, differential and integro-differential equations frequently arise which are derivable from a Lagrangian. Examples are the equations of motion of a charged particle in a time-dependent electromagnetic field; the Maxwell equations; the Vlasov-Maxwell system of equations for a collisionless plasma; and wave equations, including a large class of nonlinear wave equations. Other examples are various models of competition or conflict, such as the time-dependent Lotka-Volterra equations that describe a predator-prey system and also find application in areas such as mode coupling in plasma physics [1]. Thus, development of algorithms that provide reliable numerical solution of Lagrangian systems of equations is of considerable practical importance. In addition to requirements of accuracy, numerical stability, and speed, there is the need to capture the important qualitative features of the solutions, for example, the phase-space topology of solutions of particle equations of motion. In a many-body problem, there is the need to determine average quantities accurately, even though most details may be unimportant. For example, in the one-dimensional Vlasov-Poisson system, a quantity of particular interest is the energy of the electric field, which is an average quantity determined by the detailed motion of the many plasma particles. Usually, numerical algorithms are based directly on approximations of the governing equations. However, in the case of Lagrangian systems of equations (or their Hamiltonian equivalents), Hamilton's variational principle can be used as the basis for deriving numerical algorithms. This has the potential advantage that the numerical solutions are then based on a global principle that uniquely determines the evolution of the system. It is in contrast to attempting to mimic or preserve some particular properties of the system such as, for example, conservation of the Hamiltonian for an autonomous system, or preservation of the symplectic nature of the mapping from initial data to final data.

Hamilton's principle was introduced for deriving approximation schemes for the Vlasov-Maxwell system in 1968 [2]. Stated briefly, given a set of expansion functions for representing the spatial dependence of the electromagnetic potentials, and given a set of expansion functions for representing the dependence of the particle variables on the phase-space of their initial conditions, a system of ordinary differential equations in time was derived whose solution determines an approximation to the solution of the exact Vlasov-Maxwell system. Specialization to a collection of point particles gave particle-in-cell simulation schemes. For example, with the Vlasov-Poisson system in two cartesian spatial dimensions, if the expansion functions for the scalar potential are linear splines ("tent functions"), then this application of Hamilton's principle leads directly to the standard particle-in-cell (PIC) scheme with "area weighting."

It is well known that time-advance algorithms are very relevant to accurate plasma simulation. Indeed, Lewis, Barnes and Melendez [3] raised the question of whether a new type of time-advance algorithm could fundamentally improve the

quality of plasma simulations. The original application of Hamilton's principle to plasma simulation did not address this question; no time-advance algorithms were derived. Nevertheless, there was some belief that practical value would accrue to having time-advance algorithms based on Hamilton's principle. For example, problems with numerical stability might be avoided, or it might be possible to reduce the effects of so-called numerical collisions. Godfrey derived an algorithm to which he referred in an unpublished conference proceedings [4]. Although he found the algorithm advantageous regarding accuracy and stability, he also found it too elaborate and costly for practical use. In a later unpublished conference proceedings [5], he referred to a practicable approximate implementation of the algorithm that was sufficiently accurate for a two-dimensional PIC plasma simulation code called CCUBE. Details of the algorithms were not presented in these proceedings and the work appears not to have been pursued to examine the merits and disadvantages of time-advance algorithms based on Hamilton's principle. Eastwood has described a "virtual-particle" space-time algorithm for electromagnetic plasma simulation [6] whose derivation relies on Hamilton's principle. However, his derivation of the time-advance algorithm is inadequate because the conditions that render Hamilton's principle equivalent to specifying a particular solution of Hamilton's equations are not addressed.

Under this grant (AFOSR Grant No. F49620-92-J-0395), an initial attempt has been made to determine the properties of time-advance algorithms based on Hamilton's principle and to examine their merits and disadvantages in comparison to other approaches. The scope of the activity was limited to ordinary differential equations.

The Idea

The spirit of an initial-value problem is that of extrapolation: Initial data are to be *projected* to a later time according to the action of governing equations. However, the spirit of Hamilton's principle is that of interpolation: The solution *between* an initial time and a final time is to be determined from data at both the initial and the final times according to the action of governing equations. The key to applying Hamilton's principle to derive time-advance algorithms is realizing how to bring the extrapolatory nature of the problem into consonance with the interpolatory nature of the principle. There are two steps in using Hamilton's principle to derive a time-advance algorithm. First, a class of functions with undetermined parameters is chosen for approximating the solution of the equations over a specific time interval. For example, the approximating functions could be expansions in basis functions that are polynomials in time. This step, in one form or another, is part of any derivation of a time-advance algorithm. Second, Hamilton's principle is applied *exactly* within the class of approximating functions to obtain the conditions that the parameters must satisfy. Those conditions involve the unknown value of the solution at the final time. However, the value of the solution at the final time can be expressed in terms of the initial data and the undetermined parameters. Therefore, the conditions on the undetermined

parameters can be expressed completely in terms of the initial data. For a given class of functions used to represent approximate solutions, Hamilton's principle specifies a *unique* algorithm.

Using Hamilton's principle in a restricted function space (the space of approximating functions) is different than approximating the Lagrange or Hamilton equations of motion directly. If the function space were not restricted, then using Hamilton's principle would be equivalent to solving the exact equations of motion. However, if the function space be restricted to a set of approximating functions (for example, polynomials in time of some degree), then one may expect the approximation achieved with Hamilton's principle to be different than that obtained by applying some particular approximate method to the equations of motion directly. In fact, the algorithms based on Hamilton's principle are equivalent to a Galerkin approximation of the differential equations. Hamilton's principle determines a *particular* weight function for the Galerkin method and *constrains* the function space in which Galerkin's method is applied. The issue of which algorithms are best is complex, and it can only be resolved by detailed numerical and analytical comparison and contrast of various methods with one another.

Achievements

The following progress toward developing and understanding algorithms based on Hamilton's principle for systems of ordinary differential equations has been achieved:

- A general formulation has been developed for initial-value problems. Extensions of the formulation can be made to a wider class of problems (e.g., initial-boundary-value problems).
- Algorithms for general Lagrangians have been defined in terms of polynomial approximating functions.
- The behavior of the algorithms for small values of the timestep has been determined. It has been shown that the algorithms have a *unique* solution in the limit of zero timestep. As a result, they can be implemented in a numerically stable manner and they can be made explicit to any order in the timestep.
- If Hamilton's principle can be the starting point for deriving algorithms that are optimal in a useful sense, then the algorithms should have analogs of every general property of exact Hamiltonian and Lagrangian systems. The relation $\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$ is valid for all Hamiltonian and Lagrangian systems. For that relation, an analog has indeed been demonstrated for computational algorithms based on Hamilton's principle when the approximating functions for the coordinates and momenta are polynomials in time.

- Analytical and numerical comparisons of algorithms based on Hamilton's principle have been carried out with some other algorithms. Among the algorithms used for comparison were symplectic algorithms. Symplectic algorithms mirror Hamilton's equations in that the mapping of generalized coordinates and their conjugate momenta from one time to a timestep later is canonical, as is the case for the exact solution of Hamilton's equations. That is an appealing property, although the question of whether it is the best property to strive for is open. After all, the main objective is to approximate a *particular solution* of the equations; achieving an approximation that represents a canonical mapping as precisely as possible may or may not be valuable in the context of a particular problem. It might have been supposed that algorithms based on Hamilton's principle would also be symplectic; that is generally not the case. The comparisons of symplectic algorithms with algorithms based on Hamilton's principle indicated that the properties of the two kinds of algorithms are similar, but that the algorithms based on Hamilton's principle often approximate exact solutions better.

- Computer code using Mathematica and C has been written to enable systematic numerical comparisons of algorithms based on Hamilton's principle with some other algorithms.

In addition to the work on systems of ordinary differential equations, Hamilton's principle was used to derive a second-order accurate algorithm for the linear wave equation. It was determined that the dispersive properties of the algorithm are superior to those of the usual second-order accurate explicit or implicit algorithms. The stability restriction of the timestep is approximately the same as with the usual algorithms.

Publications

H. Ralph Lewis and Peter J. Kostelec, "Time-Advance Algorithms Based on Hamilton's Principle," paper in 10th International Workshop on Nonlinear Evolution Equations and Dynamical Systems: NEEDS '94 (September 12-16, 1994, Los Alamos, New Mexico); V. G. Makhankov, A. R. Bishop and D. D. Holm, eds. (World Scientific, Singapore, 1995); pp. 365-379.

More detailed manuscript to be submitted for publication.

Papers Presented

- 1) H. Ralph Lewis and Peter J. Kostelec, "Time-advance Algorithms based on Hamilton's Principle," paper 1D19, 1993 International Sherwood Fusion Theory Conference (March 29-31, 1993, Newport, Rhode Island).
- 2) H. Ralph Lewis, "Use of Hamilton's Principle for Numerical Approximations," Theory Seminar, Dartmouth College, Department of Physics and Astronomy, April 15, 1993.
- 3) H. Ralph Lewis, "Time-Advance Algorithms Based on Hamilton's Principle-Part I," Theory Seminar, Dartmouth College, Department of Physics and Astronomy, April 29, 1993.
- 4) H. Ralph Lewis, "Time-Advance Algorithms Based on Hamilton's Principle-Part II," Theory Seminar, Dartmouth College, Department of Physics and Astronomy, May 6, 1993.
- 5) H. Ralph Lewis and Peter J. Kostelec, "Time-advance Algorithms based on Hamilton's Principle," IEEE International Conference on Plasma Science (June 7-9, 1993, Vancouver, BC, Canada), paper 4C5-6.
- 6) H. Ralph Lewis, "Time-Advance Algorithms Based on Hamilton's Principle," Seminar, Centre National de la Recherche Scientifique (CNRS)/Physique Mathématique, Modélisation et Simulation; Orléans, France; July 2, 1993.
- 7) H. Ralph Lewis, "Time-Advance Algorithms Based on Hamilton's Principle," Colloquium, Accelerator Technology Division, Los Alamos National Laboratory, August 18, 1993.
- 8) H. Ralph Lewis, "Time-Advance Algorithms Based on Hamilton's Principle," Colloquium, Phillips Laboratory, Kirtland Air Force Base, Albuquerque, NM, August 19, 1993.

9) H. Ralph Lewis and Peter J. Kostelec, "Time-Advance Algorithms Based on Hamilton's Principle for Ordinary Differential Equations," 15th International Conference on the Numerical Simulation of Plasmas (September 7-9, 1994, King of Prussia, Pennsylvania), paper 2A1.

10) H. Ralph Lewis and Peter J. Kostelec, "Time-Advance Algorithms Based on Hamilton's Principle," 10th International Workshop on Nonlinear Evolution Equations and Dynamical Systems: NEEDS '94 (September 12-16, 1994, Los Alamos, New Mexico), presented Monday, September 12.

11) H. Ralph Lewis, "Computational Algorithms Based on Hamilton's Principle," Plasma Seminar, Dartmouth College, Department of Physics and Astronomy, November 15, 1994.